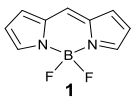
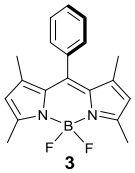
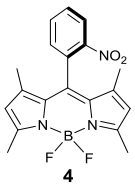
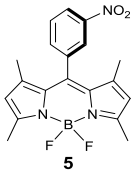
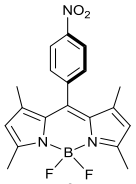
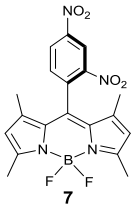
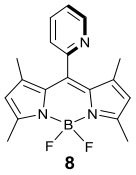
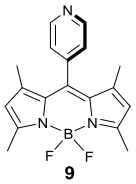
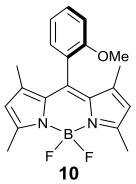
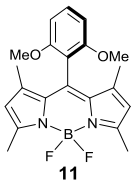
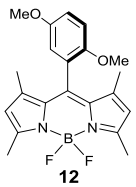
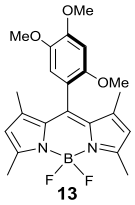
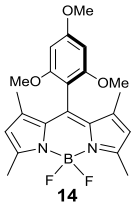
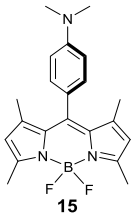
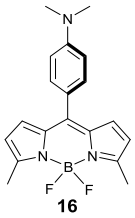
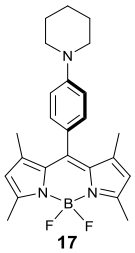
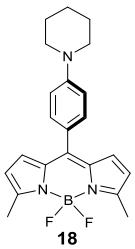
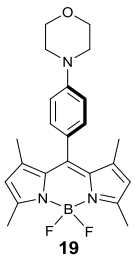
1. BODIPY dataset

Table S1. The structures and singlet oxygen quantum yield values (Φ_Δ) of heavy-atom-free BODIPYs dyes in different solvents, as searched from chemical databases. Φ_Δ values used in Models 1-3 are highlighted.

Structure	Solvent	Φ_Δ	Comment[a,b,c]	Reference
 1	hexane	0.066	A = DPIBF; S = MeSBDPI$_2$; λ_{exc} = 509 nm; [O_2] = air	1
	toluene	0.12		1
	THF	0.071		1
	MeOH	0.083		1
 2	hexane	0.03	A = DPIBF; S = MeSBDPI$_2$; λ_{exc} = 540 nm; [O_2] = air	2
	toluene	0.061		2
	CCl_4	0.100		2
	CH_2Cl_2	0.062		2
	THF	0.091		2
	EtOH	0.058		2
	CH_3CN	0.069		2
 3	hexane	0.038	A = DPIBF; S = MeSBDPI$_2$; λ_{exc} = 509 nm; [O_2] = air	3
	toluene	0.023	A = DPIBF; S = MeSBDPI$_2$; λ_{exc} = 540 nm; [O_2] = air	4
	EtOAc	0.052	A = DPIBF; S = MeSBDPI$_2$; λ_{exc} = 509 nm; [O_2] = air	3
	THF	0.13	A = DPIBF; S = MeSBDPI$_2$; λ_{exc} = 540 nm; [O_2] = air	4
	pinacolone	0.11	A = DPIBF; S = MeSBDPI$_2$; λ_{exc} = 509 nm; [O_2] = air	3
	acetone	0.050		3
	EtOH	0.030	A = DPIBF; S = MeSBDPI$_2$; λ_{exc} = 540 nm; [O_2] = air	4
	MeOH	0.031	A = DPIBF; S = MeSBDPI$_2$; λ_{exc} = 509 nm; [O_2] = air	3
	CH_3CN	0.017	A = DPIBF; S = MeSBDPI$_2$; λ_{exc} = 540 nm; [O_2] = air	4
 4	hexane	0.018	A = DPIBF; S = MeSBDPI$_2$; λ_{exc} = 509 nm; [O_2] = air	3
	EtOAc	0.027		3
	THF	0.026		3
	pinacolone	0.079		3
	acetone	0.051		3
	MeOH	0.0083		3
	CH_3CN	0.020		3
 5	hexane	0.01	A = DPIBF; S = MeSBDPI$_2$; λ_{exc} = 509 nm; [O_2] = air	3
	EtOAc	0.031		3
	THF	0.028		3
	pinacolone	0.07		3
	acetone	0.029		3
	MeOH	0.0062		3
	CH_3CN	0.0044		3
	hexane	0.0067	A = DPIBF; S = MeSBDPI$_2$; λ_{exc} = 509 nm; [O_2] = air	3
	EtOAc	0.021		3
	THF	0.019		3
	pinacolone	0.047		3
	acetone	0.0093		3
	MeOH	0.0036		3

 **6**	CH_3CN	0.0043		3
 **7**	hexane	0.021	A = DPIBF; S = MeSBDPI$_2$; λ_{exc} = 509 nm; [O_2] = air	3
	EtOAc	0.026		3
	THF	0.026		3
	pinacolone	0.073		3
	acetone	0.012		3
	MeOH	0.0055		3
	CH_3CN	0.0049		3
 **8**	hexane	0.0052	A = DPIBF; S = MeSBDPI$_2$; λ_{exc} = 509 nm; [O_2] = air	3
	EtOAc	0.0039		3
	THF	0.012		3
	pinacolone	0.012		3
	acetone	0.012		3
	MeOH	0.013		3
	CH_3CN	0.024		3
 **9**	hexane	0.0091	A = DPIBF; S = MeSBDPI$_2$; λ_{exc} = 509 nm; [O_2] = air	3
	EtOAc	0.032		3
	THF	0.024		3
	pinacolone	0.020		3
	acetone	0.031		3
	MeOH	0.012		3
	CH_3CN	0.037		3
 **10**	hexane	0.029	A = DPIBF; S = MeSBDPI$_2$; λ_{exc} = 509 nm; [O_2] = air	5
	EtOAc	0.057		5
	THF	0.061		5
	pinacolone	0.078		5
	acetone	0.17		5
	MeOH	0.021		5
	CH_3CN	0.18		5
 **11**	hexane	0.040	A[a] = DPIBF; S[b] = MeSBDPI$_2$; λ_{exc} = 509 nm; [O_2][c] = air	5
	EtOAc	0.073		5
	THF	0.051		5
	pinacolone	0.081		5
	acetone	0.082		5
	MeOH	0.036		5
	CH_3CN	0.18		5
 **12**	hexane	0.026	A = DPIBF; S = MeSBDPI$_2$; λ_{exc} = 509 nm; [O_2] = air	6
	EtOAc	0.178		6
	THF	0.462		6
	pinacolone	0.680		6
	acetone	0.250		6
	MeOH	0.023		6
	CH_3CN	0.125		6
	hexane	0.114	A = DPIBF; S = MeSBDPI$_2$; λ_{exc} = 509 nm; [O_2] = air	6
	EtOAc	0.291		6
	THF	0.357		6

 **13**	pinacolone	0.392		6
	acetone	0.068		6
	MeOH	0.004		6
	CH_3CN	0.033		6
 **14**	hexane	0.024	A = DPIBF; S = MeSBDPI$_2$; λ_{exc} = 509 nm; [O_2] = air	5
	EtOAc	0.063		5
	THF	0.059		5
	pinacolone	0.16		5
	acetone	0.11		5
	MeOH	0.074		5
	CH_3CN	0.31		5
 **15**	hexane	0.102	A = DPIBF; S = MeSBDPI$_2$; λ_{exc} = 509 nm; [O_2] = air	7
	EtOAc	0.412		7
	THF	0.623		7
	pinacolone	0.490		7
	acetone	0.114		7
	MeOH	0.073		7
	CH_3CN	0.062		7
 **16**	hexane	0.23	A = DPIBF; S = MeSBDPI$_2$; λ_{exc} = 509 nm; [O_2] = air	7
	EtOAc	0.171		7
	THF	0.321		7
	pinacolone	0.439		7
	acetone	0.087		7
	MeOH	0.019		7
	CH_3CN	0.052		7
 **17**	hexane	0.058	A = DPIBF; S = MeSBDPI$_2$; λ_{exc} = 509 nm; [O_2] = air	7
	EtOAc	0.511		7
	THF	0.612		7
	pinacolone	0.644		7
	acetone	0.145		7
	MeOH	0.037		7
	CH_3CN	0.083		7
 **18**	hexane	0.258	A = DPIBF; S = MeSBDPI$_2$; λ_{exc} = 509 nm; [O_2] = air	7
	EtOAc	0.220		7
	THF	0.401		7
	pinacolone	0.457		7
	acetone	0.099		7
	MeOH	0.046		7
	CH_3CN	0.057		7
 **19**	hexane	0.120	A = DPIBF; S = MeSBDPI$_2$; λ_{exc} = 509 nm; [O_2] = air	7
	EtOAc	0.676		7
	THF	0.535		7
	pinacolone	0.588		7
	acetone	0.192		7
	MeOH	0.038		7
	CH_3CN	0.083		7
	hexane	0.225		7